

Mathematical Physics/Numerical Analysis

# An asymptotically stable Particle-in-Cell (PIC) scheme for collisionless plasma simulations near quasineutrality

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## Abstract

We propose a new Particle-in-Cell scheme for the Vlasov–Poisson equation. This scheme remains stable when the Debye length and plasma period tend to zero without any restriction on the size of the time and length step. It relies on a semi-implicit integration of the particle trajectories. The numerical integration cost is that of the standard explicit method thanks to the use of a reformulation of the Poisson equation. *To cite this article: P. Degond et al., C. R. Acad. Sci. Paris, Ser. I 343 (2006).*

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## Résumé

**Une méthode ‘Particle-in-cell’ asymptotiquement stable pour les plasmas non-collisionnels proches de la quasineutralité.** Nous proposons un nouveau schéma ‘Particle-in-cell’ pour l’équation de Vlasov–Poisson. Ce schéma reste stable même quand la longueur de Debye et la période plasma tendent vers zéro sans restriction sur la taille des mailles spatiale et temporelle. Il repose sur une méthode d’intégration semi-implicite de la trajectoire des particules. Le coût d’intégration numérique est celui d’une méthode explicite habituelle grâce à une reformulation de l’équation de Poisson. *Pour citer cet article : P. Degond et al., C. R. Acad. Sci. Paris, Ser. I 343 (2006).*

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## Version française abrégée

De nombreux codes de physique des plasmas sont basés sur la méthode Particle-in-Cell (PIC) [1,10]. Cette méthode consiste à approcher le système de Vlasov–Poisson (1) qui décrit la théorie cinétique de particules chargées en mouvement dans leurs champs propres, à l’aide d’une discrétisation particulière (2) : voir [5,8,9]. Les simulations cinétiques de plasma sont très coûteuses en raison de la dimension importante du problème (3 dimensions d’espace et 3 dimensions de vitesse).

De plus, les simulations de plasma font intervenir des échelles multiples, liées au couplage entre les particules et les champs. Deux échelles caractéristiques de ce couplage apparaissent, la longueur de Debye  $\lambda$  (voir (1)) et la période

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plasma (qui dans l'adimensionnement choisi ici, est aussi égale à  $\lambda$ ). Ces deux échelles sont généralement très petites en comparaison des échelles de longueur et de temps caractéristiques du phénomène étudié. Aux échelles macroscopiques, le plasma peut donc être considéré comme quasineutre. Cependant, pour assurer la stabilité numérique de la méthode PIC standard, il faut assurer que la maille spatio-temporelle résolve ces deux échelles [1,10] ce qui conduit à des simulations extrêmement coûteuses.

Nous présentons une nouvelle variante de la méthode PIC qui permet des simulations stables sans que la maille spatio-temporelle n'ait à résoudre la longueur de Debye et la période plasma. Elle repose sur l'intégration semi-implicite des trajectoires des particules, solutions des équations de Newton (3). La méthode PIC standard utilise une intégration explicite de type saute-mouton (voir (4)). La nouvelle méthode consiste à utiliser la formule (5) qui présente une intégration des positions grâce à des vitesses implicites et une intégration des vitesses grâce à un champ implicite (c'est-à-dire au temps  $t^{m+1}$ ) évalué sur la position explicite (c'est-à-dire au temps  $t^m$ ) des particules. Le potentiel au temps  $t^{m+1}$  peut-être calculé grâce à une reformulation de l'équation de Poisson selon (6) que l'on discrétise implicitement (7). L'approximation spatiale est réalisée à l'aide des procédures d'assignation-interpolation standard des méthodes PIC et n'est pas détaillée ici. L'équation elliptique (7) peut être résolue au même coût que l'équation de Poisson usuelle.

Un traitement semi-implicite des trajectoires des particules a déjà été proposé dans de nombreuses références (voir en particulier [4,12–14]). Néanmoins, la présente méthode est originale. Elle a été utilisée pour la première fois dans [6,7] dans un autre contexte : celui du système d'Euler–Poisson discrétisé par volumes finis. Nous renvoyons à ces deux références pour une bibliographie plus complète.

La simulation numérique d'un cas de perturbation d'une distribution homogène de plasma démontre la stabilité uniforme de la méthode. Dans le cas où la maille spatio-temporelle résout la longueur de Debye et la fréquence plasma, on observe que la méthode PIC-AS conduit à une dissipation de l'énergie là où la méthode standard donne une bonne conservation de l'énergie totale. Nous avons observé que cette dissipation d'énergie excessive diminue après lissage de la distribution de densité (qui est très bruitée en raison de la procédure d'assignation-interpolation sur la grille).

Par contre, lorsque la maille spatio-temporelle ne résout pas la longueur de Debye ou la fréquence plasma (voir Fig. 2), la méthode standard donne des résultats totalement instables, avec des valeurs de l'énergie excédant de plusieurs ordres de grandeur les valeurs exactes. A l'inverse, la méthode PIC-AS continue de donner un ordre de grandeur correct de l'énergie.

Par conséquent, la méthode PIC-AS a le potentiel pour traiter des cas proches de la quasineutralité sans réduction drastique des pas d'espace et de temps. Néanmoins, des améliorations sont nécessaires pour réduire la dissipation d'énergie excessive de la méthode.

## 1. Introduction

Many plasma physics simulation codes are based on the Particle-in-Cell (PIC) method [1,10]. This method is an approximation method for the Vlasov–Poisson or Vlasov–Maxwell systems which describe the kinetic theory of charged particles in their self-generated field [5,8,9]. The use of kinetic models is a necessity because of the lack of collisionality of the considered plasma media which makes macroscopic fluid models invalid. As a result, collisionless plasma simulations are very expensive because kinetic equations are posed on a 6-dimensional phase-space (3 space dimensions and 3 velocity dimensions).

In addition to the high dimensionality of the problem, kinetic simulations of plasmas are complex because of the multiple scales involved. The coupling strength with the fields can be estimated by means of the Debye length and plasma period. The Debye length is a measure of the typical distance over which charge imbalances can occur and is usually very small compared with the macroscopic size of the experiment, which means that the plasma can be considered as quasineutral. The plasma period characterizes the periodic motion of the charges when a departure to quasineutrality occurs and is also usually very small compared with the typical time scales of interest.

In order to simulate the macroscopic evolution of the system, one needs to compute over a very large number of plasma periods and Debye lengths. Yet, for stability requirements of the PIC method [1,10], the Debye length and plasma period must be resolved by the numerical mesh, which requires a very large number of space and time cells. This makes PIC simulations of realistic physical phenomena computationally very demanding, in spite of many algorithmic improvements that have been developed over the years.

This Note presents a variant of the PIC method which allows stable simulations without having the space and time steps resolve the Debye length and plasma period. To our knowledge, the method is new. It relies on a semi-implicit time integration of the particle trajectories. The numerical integration cost is that of the standard explicit method thanks to the use of a reformulation of the Poisson equation. In this note, the basics of this method are outlined and some preliminary numerical simulations are given.

Semi-implicit treatments of particle trajectories have already been proposed in numerous references (see e.g. [4,12–14]). Nonetheless, the present method is different and has been first developed for the Euler–Poisson system in [6,7]. We refer to [7] and references therein for a more complete bibliography and a more detailed comparison of this method with previous ones.

## 2. The method

We only consider the one-dimensional Vlasov–Poisson system, although the method straightforwardly extends to the multi-dimensional case. We also consider only one species (the electrons) and we assume that the ions form a uniform neutralizing background. With these hypotheses, the system is written in dimensionless form:

$$\partial_t f + v \partial_x f + \partial_x \phi \partial_v f = 0, \quad \lambda^2 \partial_{xx} \phi = n - 1, \quad n = \int_{\mathbb{R}} f \, dv, \tag{1}$$

where  $f = f(x, v, t)$  is the electron distribution function depending on position  $x \in \mathbb{R}$ , velocity  $v \in \mathbb{R}$  and time  $t > 0$ ,  $\phi(x, t)$  is the electric potential and  $n(x, t)$  the electron density. The density has been normalized to the ion background density and the electron mass to unity. The dimensionless parameter  $\lambda$  is the ratio of the Debye length to the length unit, or equivalently with the normalization used, the ratio of the plasma period to the time unit.

When  $\lambda \rightarrow 0$ , the Vlasov–Poisson system is singularly perturbed and tends to a quasineutral model where  $n = 1$  everywhere. This limit has been rigorously investigated in [2]. However, using the limit model for numerical simulations leads to several practical problems. Instead, we want to propose a method which is uniformly stable when the parameter  $\lambda$  tends to zero, i.e. is not subject to time and space step constraints which tend to zero with  $\lambda$ .

The particle method consists in discretizing  $f$  into particles

$$f \approx f_N := \sum_{i=1}^N \omega_i \delta(x - X_i(t)) \delta(v - V_i(t)), \tag{2}$$

where  $N$  is the number of particles,  $\omega_i$  is a weight which must be conveniently defined at initialization (see e.g. [1,10]) and  $(X_i(t), V_i(t))$  is the location of the  $i$ -th particle in phase-space, which obeys the Newton’s equations

$$\dot{X}_i = V_i, \quad \dot{V}_i = \partial_x \phi_h(X_i, t). \tag{3}$$

The potential  $\phi_h$  is an approximation of  $\phi$ . In the PIC method, this approximation is computed on a fixed grid (be it structured or not) of space step  $h$  with a grid-defined value of the density  $n_h$ . An assignment-interpolation procedure allows to compute  $n_h$  from the location of the particles and to assign a particle value  $\partial_x \phi_h(X_i, t)$  for the field from the grid-defined potential  $\phi_h$ . This procedure is classical and is not going to be changed here (see again [1,10]).

One major issue in this procedure is the time discretization. The usual time-stepping is a ‘leap-frog’ scheme where positions are defined at integer values of the time step  $X_i^m \approx X_i(m\Delta t)$ , while velocities are defined at half-integer values  $V_i^{m+1/2} \approx V_i((m+1/2)\Delta t)$ . The integration of (3) is done as follows:

$$X_i^{m+1} - X_i^m = \Delta t V_i^{m+1/2}, \quad V_i^{m+3/2} - V_i^{m+1/2} = \Delta t \partial_x \phi_h(X_i^{m+1}, t^{m+1}). \tag{4}$$

Advancing the velocities with the second equation supposes that Poisson’s equation is solved with positions at time  $t^{m+1}$ , which is possible since these are known from the first equation. However, it is well known and widely documented in the literature [1,10] that this method suffers from a stability constraint of the form  $\Delta t, h \leq C\lambda$  where the constant  $C$  is of order of unity. We shall refer to this scheme as the standard PIC scheme.

In our method, we propose the following time-stepping strategy (where now positions and velocities are defined at integer time-steps but the method can easily be adapted to the leap-frog framework):

$$X_i^{m+1} - X_i^m = \Delta t V_i^{m+1}, \quad V_i^{m+1} - V_i^m = \Delta t \partial_x \phi_h(X_i^m, t^{m+1}). \tag{5}$$

The positions are advanced with implicit velocities, but more importantly, the velocities are advanced with an *implicit field* (i.e. at time  $t^{m+1}$ ) evaluated at the *explicit positions* of the particles (i.e. at time  $t^m$ ). Computing with an implicit field can be done easily, with not more computational effort than with an explicit method. In order to do this, we use a reformulation of the Poisson equation which is described below (see also [6,7]).

Using the continuity and momentum conservation equations that can be deduced by taking the moments of the Vlasov equation (1), and after a few algebraic manipulations (see [6,7]), we find that the following *reformulated Poisson equation*:

$$-\partial_x((n + \lambda^2 \partial_{tt})\partial_x \phi) = -\partial_{xx} S, \quad S = \int f v^2 dv, \quad (6)$$

is equivalent to the original one provided that the Poisson equation (and its time derivative) are satisfied initially. Now, the implicit potential  $\phi(x, t^{m+1})$  is found by a semi-implicit time differencing of (6):

$$-\partial_x((n^m \Delta t^2 + \lambda^2)\partial_x \phi^{m+1}) = -\Delta t^2 \partial_{xx} S^m - 2n^m + n^{m-1} + 1. \quad (7)$$

The spatial approximation of (7) is done in the usual way, by discretizing it on a fixed grid. The only difference with using the usual Poisson equation (from the computational view point) is the need to construct grid values of the pressure tensor  $S$  by the assignment procedure.

The elliptic equation (7) can be solved at the same cost as the usual Poisson equation. The only additional cost is the assignment of  $S$ . Although this cost can be large (because the assignment-interpolation routine is expensive as compared with the other parts of a PIC method) it is far more than compensated by the possibility of using large time steps, irrespective of the smallness of  $\lambda$ , as will be demonstrated by the numerical simulations below. Therefore, the expected CPU saving is large. We shall refer to the scheme as the AS-PIC scheme (AS = asymptotically stable).

Although this method bears some analogies with previously proposed methods, it does not reduce to any of them. The direct implicit method [4,12] uses a modified Poisson equation with an 'implicit dielectric susceptibility'. In our method, the right-hand side is not the charge density, but the Hessian of the pressure tensor. In the implicit moment method [13,14], the continuity and momentum equations are used, but Poisson's equation is replaced by Ampere's equation.

### 3. Numerical results

Our test problem is the perturbation of a Maxwellian plasma. We initialize the Vlasov–Poisson equation with  $f_0(x, v) = \pi^{-1/2}(1 + \delta \sin(\kappa \pi x)) \exp(-v^2)$ , on the interval  $[0, 1]$  with periodic boundary conditions. If  $\delta \ll 1$ , the solution can be computed by linearization [3,11] and consists of Landau-damped plasma waves. The particle initialization is done by random sampling. As a diagnostic, we look at the electrostatic, kinetic and total energies  $E_p$ ,  $E_k$  and  $E_t$  respectively given by

$$E_p = \frac{\lambda^2}{2} \int |\partial_x \phi|^2 dx, \quad E_k = \frac{1}{2} \int f |v|^2 dx dv, \quad E_t = E_p + E_k. \quad (8)$$

The total energy is conserved in the course of time.

In Fig. 1, we first compare the standard and AS-PIC scheme when the mesh step resolves the Debye length ( $h = \lambda = 10^{-2}$ ). We notice that the AS-PIC scheme damps out the total energy. This energy loss is a point to which future work has to be devoted.

In Fig. 2, we compare the standard and AS-PIC scheme when the mesh step does not resolve the Debye length:  $h = 10^{-2}$ ,  $\lambda = 10^{-4}$ . The standard PIC scheme becomes instantaneously unstable, with a total energy reaching  $10^4$  times its initial value after one time-step. In the AS-PIC scheme, the energy remains bounded by its initial value and decreases with time. Simultaneously, we have checked that the time step (which is computed through the CFL condition  $v_{th} \Delta t \leq \Delta x$  where  $v_{th}$  is the thermal velocity of the distribution), reaches values which are about a hundred times the plasma period.

The strong decay of the energy in the AS-PIC scheme has been attributed to the large noise (resulting from the PIC assignment procedure) in the coefficients of the Poisson equation (7). By filtering out this noise (cutting out the high frequencies), we have observed that the energy decay can be strongly reduced. More work has to be done to reduce this spurious energy decay.

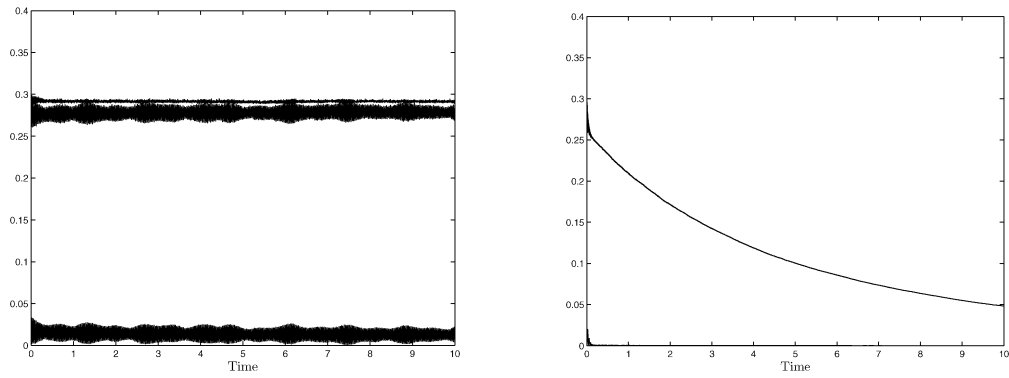


Fig. 1. The Debye length and plasma period are resolved. Left: standard PIC scheme; right: AS-PIC scheme. From bottom to top curves: electrostatic, kinetic and total energies (scale = 0.05 dimensionless unit (DU)) as functions of time (scale = 1 DU). On the right figure, the bottom curve is almost confounded with the horizontal axis (except in the lower left corner) and the two top curves are confounded.

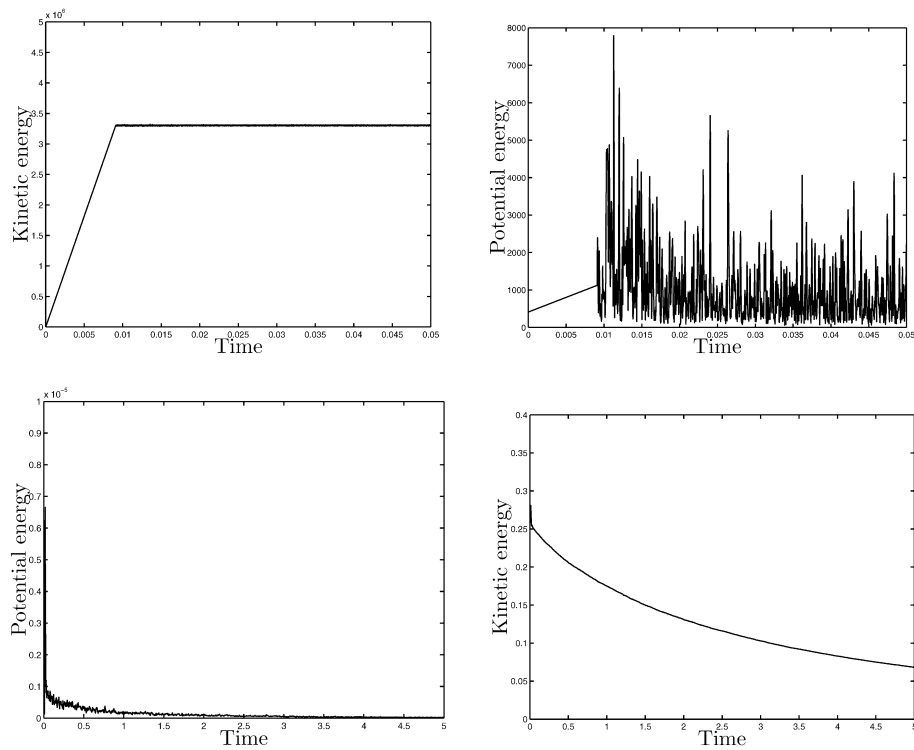


Fig. 2. The Debye length and plasma period are unresolved. Left and middle left: standard PIC scheme (left: electrostatic energy (scale =  $5 \times 10^5$  DU); right: kinetic energy (scale =  $10^3$  DU)); middle right and right: AS-PIC scheme (left: electrostatic energy (scale =  $10^{-6}$  DU); right: kinetic energy (scale =  $5 \times 10^{-2}$  DU)) as functions of time (time scale for the standard PIC simulations =  $5 \times 10^{-3}$  DU and for the AS-PIC simulations =  $5 \times 10^{-1}$  DU).

#### 4. Conclusion

We have presented a novel PIC method for kinetic simulations of plasmas. The method allows us to treat quasineutral regimes without a drastic reduction of the time and space meshes. A first set of numerical simulations has been done which demonstrates the potential of the method and identifies the points which require further investigations (among which is a too strong energy dissipation). More numerical simulations and improvements are in progress.

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